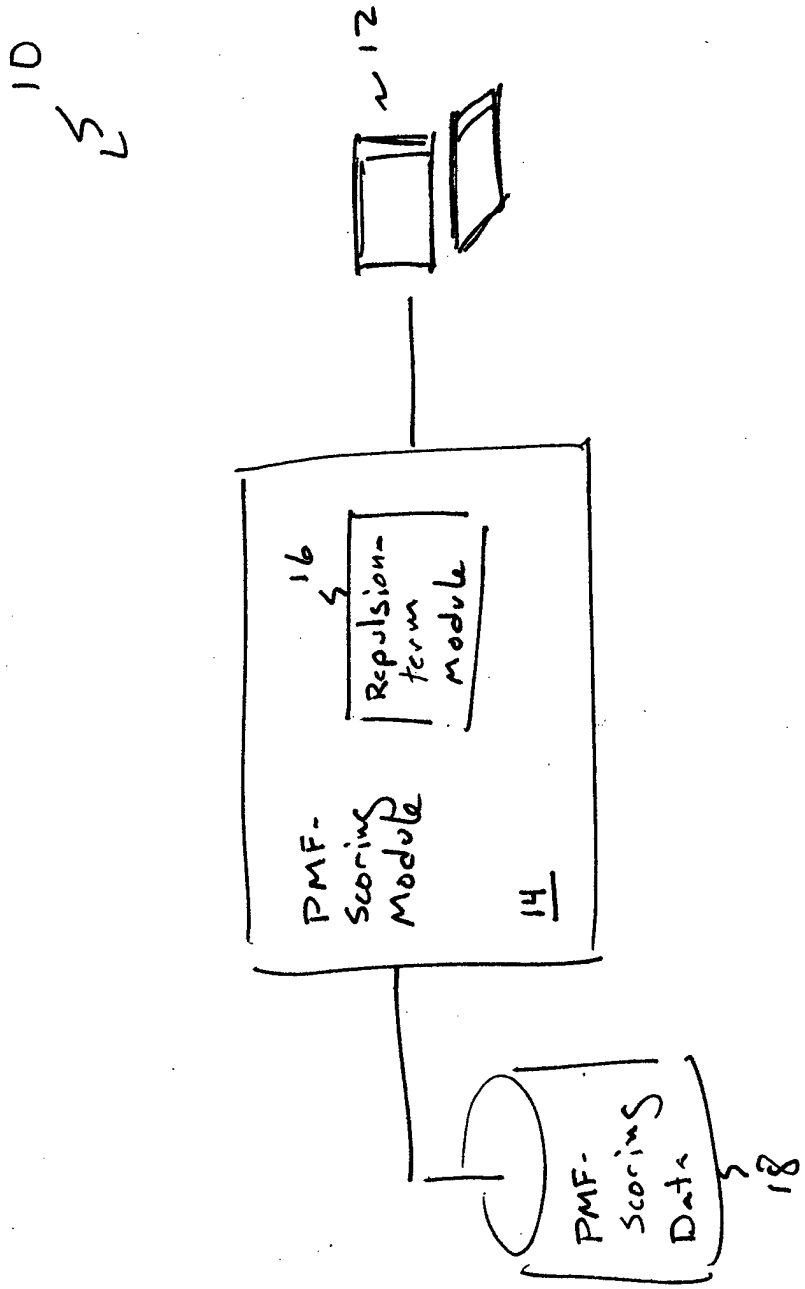
10
12
16
Repulsion term Module
PMF-scoring Module
14
PMF-scoring Data
18

Figure 1

30

	32a Atom-Pair Type	32b Distance Value (Angstroms)	32c Well-Depth Value (-kcal/mol)
34a	CF-CO	4.2	0.1917
34b	CF-CN	4.2	0.3797
34c	CF-NC	3.55	0.4225
34d	CF-NP	4.2	0.3025
34e	CP-OA	3	0.4325
34f	NC-CO	3.8	1.4381
34g	OC-OD	2.6	1.4604
34h	OA-ND	2.9	0.7225
34i	SA-NR	4.4	0.6577

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Figure 2

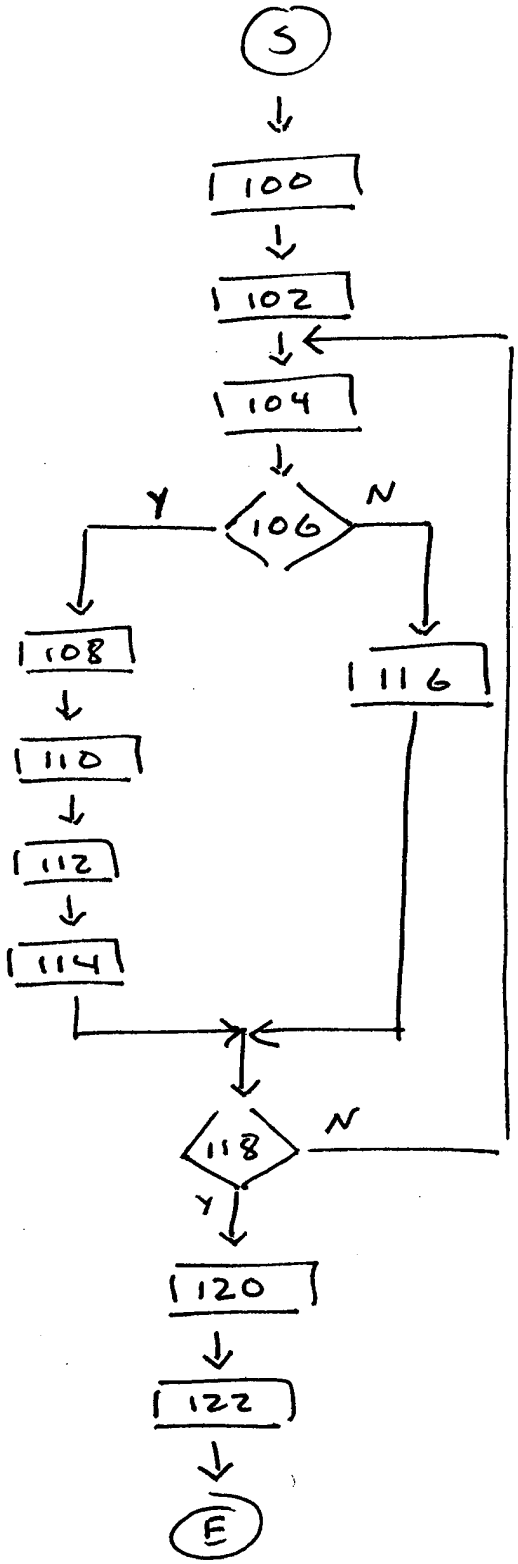

Figure 3

100. USER SPECIFIES PROTEIN-LIGAND COMPLEX

102. PMF-SCORING MODULE ACCESSES PMF-SCORING DATA ASSOCIATED WITH SPECIFIED PROTEIN-LIGAND COMPLEX

104. PMF-SCORING MODULE IDENTIFIES PROTEIN-LIGAND ATOM PAIR IN SPECIFIED PROTEIN-LIGAND COMPLEX

106. SHOULD REPULSION TERM BE USED TO CALCULATE PMF OF IDENTIFIED PROTEIN-LIGAND ATOM PAIR?

108. PMF-SCORING MODULE ACCESSES TABLE OF EMPIRICALLY DERIVED MINIMUM BINDING-ENERGY DISTANCE AND WELL-DEPTH VALUES

110. PMF-SCORING MODULE USES ACCESSED TABLE TO DETERMINE A MINIMUM BINDING-ENERGY DISTANCE VALUE AND A WELL-DEPTH VALUE THAT CORRESPOND TO IDENTIFIED PROTEIN-LIGAND ATOM PAIR

112. PMF-SCORING MODULE USES DETERMINED MINIMUM BINDING-ENERGY DISTANCE AND WELL-DEPTH VALUES TO CALCULATE REPULSION TERM

114. PMF SCORING MODULE USES CALCULATED REPULSION TERM TO CALCULATE PMF OF IDENTIFIED PROTEIN-LIGAND ATOM PAIR

116. PMF SCORING MODULE CALCULATES PMF OF IDENTIFIED PROTEIN-LIGAND ATOM PAIR WITHOUT REPULSION TERM

118. PMF CALCULATED FOR EVERY PROTEIN-LIGAND ATOM PAIR IN SPECIFIED PROTEIN-LIGAND COMPLEX?

120. PMF-SCORING MODULE USES CALCULATED PMFs TO CALCULATE PMF SCORE OF SPECIFIED PROTEIN-LIGAND COMPLEX

122. PMF-SCORING MODULE COMMUNICATES CALCULATED PMF SCORE TO USER

Figure 3 (continued)